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A USERS' GUIDE TO THE TRACE CONTAMINANT CONTROL SIMULATION COMPUTER PROGRAM

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The Trace Contaminant Control Simulation computer program is a tool for assessing the performance of various trace contaminant control technologies for removing trace chemical contamination from a spacecraft cabin atmosphere. The results obtained from the program can be useful in assessing different technology combinations, system sizing, system location with respect to other life support systems, and the overall life cycle economics of a trace contaminant control system. The user's manual is extracted in its entirety from NASA TM–108409 to provide a stand-alone reference for using any version of the program. The first publication of the manual as part of TM–108409 also included a detailed listing of version 8.0 of the program. As changes to the code were necessary, it became apparent that the user's manual should be separate from the computer code documentation and be general enough to provide guidance in using any version of the program. Provided in the guide are tips for input file preparation, general program execution, and output file manipulation. Information concerning source code listings of the latest version of the computer program may be obtained by contacting the author.

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A USERS' GUIDE TO THE TRACE CONTAMINANT CONTROL SIMULATION COMPUTER PROGRAM

USERS' GUIDE BACKGROUND

The Trace Contaminant Control Simulation (TCCS) computer program was first documented in "Computerized Atmospheric Trace Contaminant Control Simulation for Manned Spacecraft," NASA TM–108409 in June 1993. The users' guide portion of that technical memorandum has been extracted and reproduced here since future changes and upgrades to the computer program source code require the documentation to be revised periodically. By separating the users' manual from the documentation for the latest version of the computer code, the existence of multiple versions of the users' guide can be avoided. The following guide has been extracted in its entirety from TM–108409.

INTRODUCTION TO TRACE CONTAMINANT CONTROL

Buildup of atmospheric trace contaminants in enclosed volumes such as a manned spacecraft may lead to potentially serious health problems for the crewmembers. For this reason, control methods are implemented to minimize the concentration of atmospheric contaminants to levels that are considered safe for prolonged, continuous exposure. Methods employed to achieve these levels are classified into two major categories—passive and active. Passive control refers to the material selection and control process to which all bulk materials and assembled articles must be subjected to qualify for flight onboard a manned spacecraft. Criteria included in this process are flammability, odor, and offgassing characteristics. Through this screening, the uncontrolled production via offgassing mechanisms of atmospheric contaminants from materials used in the habitable areas of the spacecraft are limited, but not eliminated. Active control methods must be used to provide the second level of contaminant control. Activities such as food preparation, housekeeping, and personal hygiene contribute to the base contamination load found in the spacecraft atmosphere. Contaminants also are produced by crewmember metabolism, experiment hardware and operations, and spacecraft hardware operations. The activities onboard the spacecraft combined with material offgassing produce contaminants in sufficient quantities that the atmospheric concentration may build up to levels which the crewmembers may find irritating or possibly intolerable. Therefore, the total contamination control approach requires both the passive and active approaches.

Active contamination control can be achieved through various means. Typical technologies used onboard manned spacecraft include physical adsorption on granular activated charcoal or other adsorbent material, chemical adsorption using impregnated granular activated charcoals and granular lithium hydroxide (LiOH), ambient temperature catalytic oxidation, and high temperature catalytic oxidation. Other means which are significant include removal by absorption into humidity condensate and spacecraft atmospheric leakage. These latter methods are not specifically designed to remove atmospheric contaminants but have been shown to be significant when the total contaminant material balance in a spacecraft is considered.

Designs for active contamination control hardware have evolved from single granular activated charcoal canisters used onboard earlier manned spacecraft, to a regenerable molecular sieve adsorbent used onboard the Skylab orbital workshop. Space shuttle and Spacelab programs use layered adsorbent canisters containing nonregenerable adsorbent and ambient temperature catalytic oxidation materials. Future contamination control hardware will build on these technologies to include regenerable adsorbent materials and high temperature oxidation catalysts.

Designing these contamination control devices is difficult since they must be designed without thorough knowledge of the overall load that must be controlled. Historical data from past manned missions are important for understanding the loads from offgassing, crew metabolism, and housekeeping sources. This information forms the basis for a generic spacecraft load model which can be used for hardware design purposes. As the spacecraft design matures, the contamination control hardware is refined by replacing the load model data with data for the actual flight hardware. Ultimately, the spacecraft and contamination control designs converge. The final result is a robust contamination control hardware design with sufficient margin which allows a wide range of hardware and activities to be accommodated onboard the spacecraft with no adverse effects on the crewmembers' health.

COMPUTER SIMULATION BACKGROUND

In the past, designing contamination control hardware required extensive testing to characterize and select the appropriate control technologies. Capacities for granular activated charcoal and other adsorbent materials had to be determined along with development of theoretical approaches to predicting the performance of future contamination control hardware. Early efforts to select technology and design hardware for spacecraft contamination control hardware began during the *Apollo* project. Studies conducted before 1965 by Lockheed Missiles and Space Company in Sunnyvale, CA, developed early spacecraft contaminant load models and selected candidate technologies.[1 2 3] These technologies have been the basis for designing contamination control hardware for manned spacecraft ever since. More detailed studies on adsorption and catalytic oxidation followed. High temperature catalytic oxidation was studied by Olcott[4] and contaminant adsorption by Robell et al.[5] by late 1970. In his work, Robell developed an extremely useful correlation for predicting the loading capacity of granular activated charcoal by using the potential theory developed by Polanyi.[6] This work became the basis for computer simulation of adsorption processes to be used onboard manned spacecraft for atmospheric contamination control. The first generation simulation program was developed by Olcott before May 1972 using the technique developed by Robell.[7] By 1975, a prototype contamination control system had been fabricated by Lockheed, and the first generation computer simulation program for adsorption had been used under NASA contract NAS 1–11526 to analyze the hardware performance.[8]

Work continued in characterizing contamination control technologies, and low temperature oxidation catalysts were studied in 1977. That same year, the first integrated computer simulation model for spacecraft atmospheric contamination control was developed by Jagow et al. at Lockheed.[9] This program was specifically tailored for analyzing the performance of the Spacelab contamination control canister which consisted of two layers of adsorbent material followed by a layer of low temperature carbon monoxide oxidation catalyst. This program was modified and released later in 1977 as a general computer simulation program capable of simulating any spacecraft contamination control system given the appropriate input data.[10] This basic computer program was used for design and preflight performance analyses for Spacelab missions.

Little work was conducted on the basic computer program until NASA contract NAS8–36406 produced a new release of the computer program in 1986 which featured input data manipulation using commercially available spreadsheet software and operation on a personal computer. This program version, designated version 5.0, was used as the basis for Space Station *Freedom* contamination control hardware design.[11] Improvements since 1986 have included further enhancements for input data manipulation, a routine to calculate the toxic hazard index, improved simulation of humidity condensate absorption, updated charcoal equilibrium loading equations, and improved output data manipulation flexibility. Written in FORTRAN 77, the program can be run on IBM-compatible personal computers (version Alpha) and Apple Computer, Inc., Macintosh™ computers (version Gamma).

SIMULATION PROGRAM OVERVIEW

Computer Hardware Requirements

The TCCS computer program version Alpha is written in FORTRAN 77 and can be run on personal computers using 80286, 80386, 80486, or Pentium™ microprocessors. The computer should be operating under Disk Operating System (DOS) version 3.0 or higher for program execution and data file preparation. To obtain maximum performance from the program, a math coprocessor chip is recommended. At least 512 kb of memory are necessary for program execution. Upgraded personal computers using the 80386, 80486, or Pentium processors are preferred since they provide more rapid execution. The program is compiled and linked on the personal computer using Ryan-McFarland FORTRAN version 2.42.

A second version (Gamma) of the TCCS computer program, which runs on Apple Computer, Inc. Macintosh™ machines, is available and operates similarly to the DOS-supported version. The Macintosh™ user interface, which uses a mouse and pop-up menus for input file management, makes the program even more user-friendly by requiring fewer commands to be entered from the keyboard. It is recommended that this version be run on at least a Macintosh™ II family machine with 8 megabytes of random access memory (RAM) and Macintosh™ Operating System version 7.0.

Input/Output Data Manipulation Recommendations

Input data are manipulated using commercially available spreadsheet software. The program can read input data using both space- and comma-delimited formats, while output data is produced in a space-delimited ASCII format. Because of these program input and output data formats, it is recommended that the Lotus Development Corporation (Lotus) software Lotus 1-2-3™ with Printgraph™ or Microsoft Corporation's Excel™ be used for input data generation and output data manipulation for the personal computer version. This software can print to a file in the space-delimited or comma delimited ASCII format required by the program and import program output data directly without any additional processing by the user. When using Lotus 1-2-3™, input files should be saved by using the print-to-file utility. Input files built using Excel™ should be saved in the comma separated variable (CSV) format. Other spreadsheet programs may be used as long as ASCII files in the space and comma-delimited formats are available as options.

The Macintosh™-supported version of the program should use the Microsoft Corporation Excel™ spreadsheet software for input file preparation and output data analysis. Input files prepared using Excel™ must be saved as a CSV file for the program to read the data. Output data produced by the

program may be imported into the Excel™ spreadsheet and then the parse function run to place each number in a spreadsheet cell. Data plots may be prepared using Excel™ or the data may also be loaded into other popular Macintosh™ plotting software such as Cricket Graph™ or Kaleidograph™.

Calculation Overview

The TCCS program calculates the cabin concentration of specified contaminants given a set of contamination control devices as a function of time. Depending on the output data selections made, data for each basic time increment may be output detailing the current contaminant cabin concentrations, their comparison to the spacecraft maximum allowable concentrations (SMAC's), the removal rate for each contaminant in each device, the cumulative total contaminant mass removed by each device, the increment device single pass removal efficiency for each contaminant, and the toxic hazard index.

Input Data

Input information consists of the names and properties of each contaminant, the order and design characteristics of the removal devices, and time-dependent data such as changes in contaminant generation rate or removal device flow rate as a function of time. These input data are read into the program using three separate data files. The first file contains contaminant data, the second contains removal device definition data, and the third contains time-dependent data. Files are used for input to minimize repetitive input by the user.

Contaminant Removal Devices

Removal device configuration is provided by a routine which allows up to 15 total devices with parallel and series arrangement. Up to three devices in parallel can be placed upstream of any removal device. The program simulates nine removal device types. Two device types, the cabin and leakage, must always be included in the device definition file. Modular programming allows for quick revision or addition of device types if necessary; however, any internal modifications require recompiling and relinking the program.

Calculation Convergence

A discrete time increment approach is used by the program which uses contaminant concentration from the previous increment as the initial concentration. The final concentration is calculated based on the device configuration, contaminant generation rate, contaminant removal rate, removal device efficiency, and other specific information relevant to that time increment. This approach allows flexibility which simulates transient situations such as inadvertent contaminant releases or other time-dependent contamination events. The calculation data are stored in matrices which increase the program execution speed.

Since contaminant properties can vary with respect to ease of removal and cabin concentration, small time increments would be the most accurate for any given simulation. However, the program uses a log-mean direct solution approach combined with a Newton-Raphson convergence routine to allow much larger time increments which significantly reduce the computer runtime required. This approach produces an exact solution during steady-state conditions with constant removal device efficiencies. This is normally the case during a simulation. But efficiency may vary in some cases, such as for a contaminant that is breaking through an adsorbent bed. In this case, the Newton-Raphson convergence technique

combined with decreasing the time increment to one-tenth the size of the basic increment for that contaminant only provides the desired calculation accuracy without affecting the overall run time.

The prediction and convergence routines use the Newton-Raphson technique to ensure that the removal device calculations are made with the proper contaminant inlet concentration. Contaminant concentrations are predicted using the removal efficiencies of the previous increment and the generation rates for the present increment. Actual device efficiencies and contaminant concentrations are calculated by the convergence routine and compared to the predicted values. This process continues until the predicted and calculated values agree within a specified error.

If convergence is not obtained for a contaminant, warning statements built into the program alert the user. In addition, other warning statements concerning input and output are provided to aid simulation diagnostics. Print options are provided to allow printing the contents of calculation matrices and convergence values. These options allow quick identification of problems with the input device configuration or contaminant data.

Output Data

Program output data consist of standard formatted output with column headings and page numbers and interactive formatted output to files for data plotting. Standard formatted data output is specified using print switches in the device definition input file, while plot data output is specified interactively. Standard output consists of the contaminant name, cabin concentration, SMAC, and a designation of whether the cabin concentration exceeds the SMAC. Also, the standard print switches allow the contaminant removal rate, cumulative mass removed, and removal efficiencies for each contaminant in each device to be output. Standard output may be directed to the computer terminal screen, a specific data file, or a printer. These data include page numbers, time increment identification, and other information relating to the time increment. Interactive output decisions are made by the user to produce separate files containing concentration, device efficiency, and toxic hazard index data as a function of time. These files are in a spreadsheet format and can be imported to a spreadsheet to allow manipulation and preparation of data plots. The toxic hazard index is also interactively sent to the standard formatted output in addition to a plot file if desired.

PROGRAM OPERATION

The computerized atmospheric trace contaminant control simulation program requires 33 FORTRAN 77 routines. Figure 1 shows a block flow diagram of a simulation of an atmospheric contamination control case. An operation description for using this program includes instructions for preparing input data files and operating the program.

Input Data File Preparation

Before program operation, three input files must be prepared to define the contaminant properties and generation rates, removal device configuration, and time-dependent inputs. These files are created using commercially available spreadsheet software which is capable of producing space delimited ASCII files. Lotus 1-2-3™ is the preferred spreadsheet program for creating these input files. The print-to-file option in Lotus is used to send the appropriate data range to each file. These files are read by the program and the data are placed into calculation matrices NN, CDI, DD, and TT. Matrix NN is

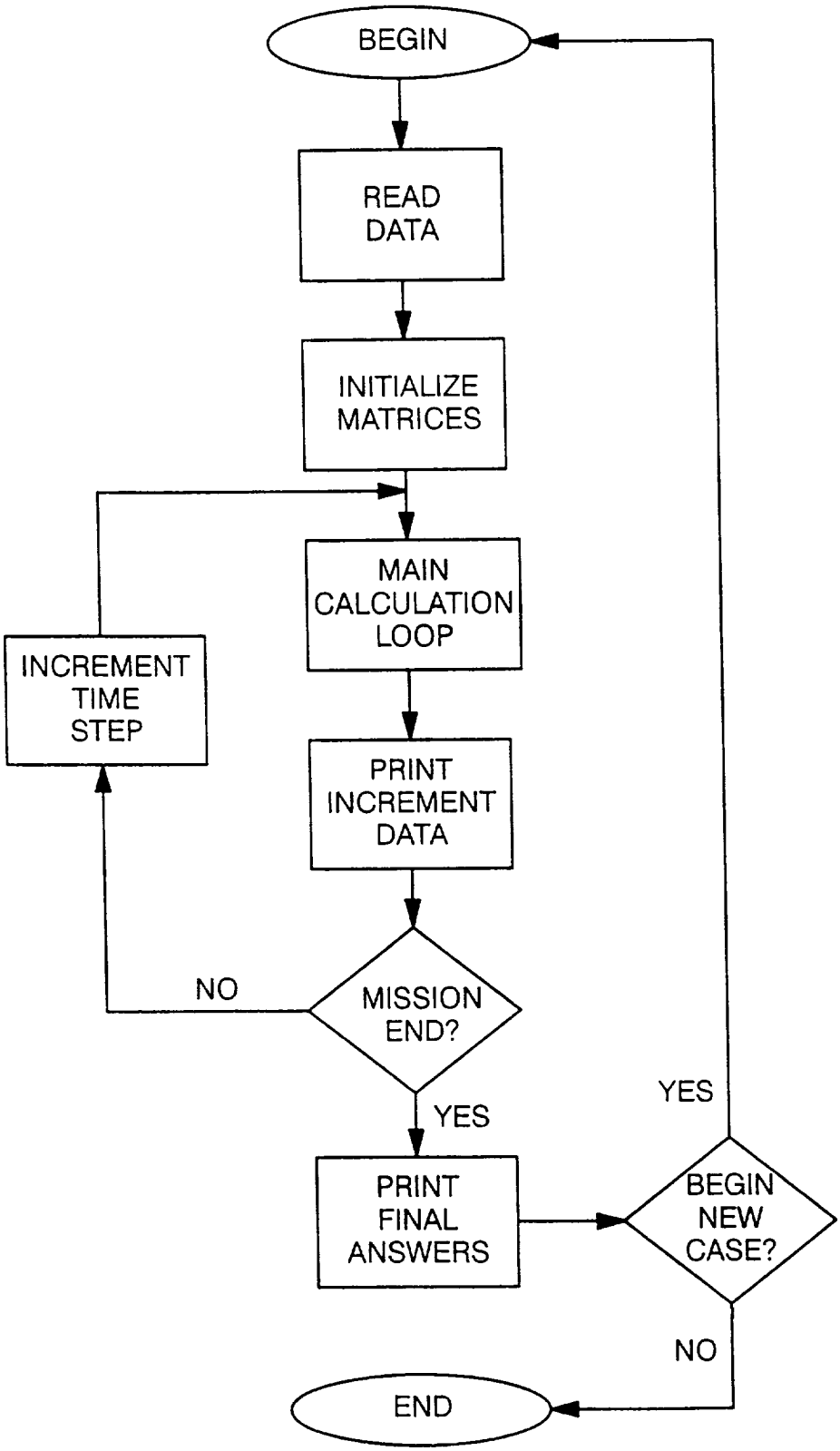


Figure 1. Simplified computer program flow chart.

a 1 by 300 matrix containing the contaminant names, CDI is a 23 by 300 matrix containing contaminant physical properties defined in table 1, matrix DD is a 15 by 22 matrix containing removal device design and configuration data defined in tables 2 and 3, and matrix TT is a 7 by 750 matrix containing time-dependent contaminant generation rate and device flow rate data. The matrix sizes are adjustable; however, the personal computer version is limited to 300 contaminants so that the contaminant matrix does not exceed 64 kb to provide a more rapid run time.

Table 1. Required contaminant physical properties and generation data.

Contaminant Property	Units and Remarks
Contaminant name	30 character maximum
Cabin generation rate	mg/h
Liquid density	gm/cm^3 (cabin conditions)
Molar volume	cm^3/g-mol (cabin conditions) (0 = no charchoal removal)
Molecular weight	gm/g-mol
Vapor pressure	mg/m^3 (cabin conditions)
Henry's Law constant	atm/mol-fraction
Lithium hydroxide removal	lb_m LiOH/lb_m contaminant removed (0 = no removal)
Chemical category	According to NHB 8060.1B Appendix D
Maximum allowable concentration	mg/m^3
Generation rate in devices 3 to 15	mg/h
Degree of oxidation in a high-temperature oxidizer	0 = none; 1 = fully

Contaminant Data Input File Preparation

The contaminant data input file contains the contaminant names, physical properties, generation rates in the cabin and each device, and the degree of oxidation in a high temperature catalytic oxidation process. These data are read into program calculation matrices NN and CDI. Sample input is shown in figure 2. Data required for each column of the contaminant data input file are the following:

1. The contaminant sequential number, 1 through 300

2. An apostrophe to enclose the contaminant name as required by FORTRAN 77

Table 2. Example device definition table.

TCCS PROGRAM INPUT DATA
DEVICE DEFINITION TABLE

USE RANGE 'LIST' DATA TABLE TO PRINT TO PRINTER
USE RANGE 'DATA' TO PRINT DATA TO FILE

MATRIX COLUMN NO. 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
DEVICE NO.	DEVICE FLOW (m3/h)	DEVICE TYPE NO.	UPSTREAM DEVICES BY NUMBER NO.1	NO.2	NO.3	NOT FOR INPUT	COL 8 TO 16 USED FOR DEVICE SPECIFIC INPUTS SEE TABLE BELOW								
1	0.00	1	0	0	0	0	0	227.86	293	24	1.00E-01	1.2	0	0	0
2	0.0460	2	1	0	0	0	1	0	0	0	0	0	1	1	0
3	519.90	8	1	0	0	0	1	1.451	0	0	0	0	0	0	0
4	15.12	3	1	0	0	0	1	0.580	0.320	0	490	2	0	0	0
5	4.08	7	4	0	0	0	1	0.000	0.000	0	0	0	0	0	0
6	4.08	5	5	0	0	0	1	0.234	0.129	0	442	0	0	0	0

Table 3. Device definition data by device type for data table columns 8 through 16.

Device Number	Device Type	Device Definition Table Column Number								
		8	9	10	11	12	13	14	15	16
1	Cabin	0	Volume (m^3)	Temperature (K)	Time Increment (h)	Converge Error (decimal)	Coexist Factor (1.20)	Relative Humidity (Percent)	0	0
2	Leakage	1	Print Switch No.1	Print Switch No.2	Print Switch No. 3	Print Switch No. 4	Print Switch No. 5	Print Switch No. 6	Print Switch No. 7	Print (3) Switch No. 8
3	Axial Charcoal	Maximum Efficiency (decimal)	Bed Length (m)	Bed Diameter (m)	0	Matl. Bulk Density (kg/m^3)	Bed Treatment Type (4)	Regeneration Data		
								First (h)	Interval (h)	Duration (h)
4	Radial Charcoal	Maximum Efficiency (decimal)	Bed Length (m)	Bed Outside Diameter (m)	Bed Inside Diameter (m)	Matl. Bulk Density (kg/m^3)	Bed Treatment Type (4)	Regeneration Data		
								First (h)	Interval (h)	Duration (h)
5	LiOH Bed	Maximum Efficiency (decimal)	Bed Length	Bed Diameter (m)	0	Matl. Bulk Density (kg/m^3)	Changeout Data		0 (1)	0 (2)
							First (h)	Interval (h)		
6	CO Oxidizer	Maximum Efficiency (deciman)	Bed Length (m)	Bed Diameter (m)	0	0	0	0	0	0
7	Catalytic Oxidizer	1	0	0	0	0	0	0	0	0
8	Condensing Heat Exchanger	1	Condensate Flow (kg/h)	0	0	0	0	0	0	0
9	Dummy Device	0	0	0	0	0	0	0	0	0

NOTES:
1. Used to store total weight of LiOH used in the calculation in kg/h
2. Used to store total weight of LiOH used during the calculation in kg
3. Print switches are set to 1 for printing and 0 for no printing. No. 1 to 5 for diagnostics, 6 to 8 for printout.
4. 0 = no treatment; 1 = chromate treatment for formaldehyde; 2 = phosphoric acid treatment for ammonia.

CONTAMINANT INPUT DATA TABLE (Spacelab Missions 1 and 3 basis using maximum generation rates)

MAKE SURE ALL CELLS HAVE A VALUE OR 0 IN CELL

CONT NO.	NAME(30 CHR MAX)	CABIN RATE mg/h	LIQUID DENSITY g/cc	MOLAR VOL cc/mol	MOLAR MASS g/mol	VAPOR CONC mg/m3	H2O SOL HENRY atm,0=i	LIOH lb LiOH/ lb cont	NHB 8060.1B GROUP	SMAC mg/m3	GENERATION IN DEVICES 3 THROUGH 15 mg/h													OXIDIZER EFF decimal
1	1,1,2-triCl-1,2,2-triFlethane	279.99	1.564	120.0	187.40	3280000	2.69E+04	0	7	383.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0.33
2	1,3-Butadiene	0.06	0.676	82.0	54.09	7047000	2.42E+03	0	9	221.20	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
3	Methane	30.81	0.425	37.7	16.04	225400000	3.54E+04	0	9	1771.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0.95
4	2-butanone	45.81	0.805	96.7	72.11	405400	1.63E-01	0	11	59.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
5	1-benzo[b]pyrrole	1.04	1.220	139.8	117.15	74	2.48E-02	0	15	0.48	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
6	methyl hydrazine	0.03	0.875	63.0	46.07	1233000	2.70E-02	0	15	0.08	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
7	Ammonia	53.49	0.639	25.0	17.00	7522000	9.37E-01	0	16	17.40	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
8	Carbon monoxide	24.04	0.803	22.1	28.01	974700000	6.34E+04	0	16	28.60	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
9	Hydrogen	4.65	0.071	3.0	2.02	2033000	6.52E+04	0	16	247.30	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00

CONTAMINANT INPUT DATA FILE EXAMPLE

1,1,2-triCl-1,2,2-triFlethane	279.99	1.564	120.0	187.40	3280000	2.69E+04	0	7	383.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0.33
1,3-Butadiene	0.06	0.676	82.0	54.09	7047000	2.42E+03	0	9	221.20	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
Methane	30.81	0.425	37.7	16.04	225400000	3.54E+04	0	9	1771.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0.95
2-butanone	45.81	0.805	96.7	72.11	405400	1.63E-01	0	11	59.00	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
1-benzo[b]pyrrole	1.04	1.220	139.8	117.15	74	2.48E-02	0	15	0.48	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
methyl hydrazine	0.03	0.875	63.0	46.07	1233000	2.70E-02	0	15	0.08	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
Ammonia	53.49	0.639	25.0	17.00	7522000	9.37E-01	0	16	17.40	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
Carbon monoxide	24.04	0.803	22.1	28.01	974700000	6.34E+04	0	16	28.60	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00
Hydrogen	4.65	0.071	3.0	2.02	2033000	6.52E+04	0	16	247.30	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00

NOTE: THE CONTAMINANT INPUT DATA FILE IS CREATED BY WRITING THE SELECTED RANGE TO A FILE FROM THE SPREADSHEET. THIS FILE IS IN ASCII FORMAT. THE CONTAMINNAT NUMBER IS NOT SELECTED FOR THE INPUT DATA FILE.

Figure 2. Sample contaminant input data table and input file.

3. The contaminant name up to 30 characters

4. An apostrophe to enclose the contaminant name as required by FORTRAN 77

5. The contaminant cabin generation rate in milligrams per hour (mg/h)

6. The contaminant liquid phase density in grams per cubic centimeter (g/cm^3)

7. The contaminant molar volume in cubic centimeters per gram-mole ($cm^3/g\text{-}mol$)

8. The contaminant molecular weight in grams per gram-mole (g/g-mol)

9. The contaminant vapor pressure at the cabin temperature expressed in milligrams per cubic meter (mg/m^3)

10. The water solubility for the contaminant expressed as the Henry's Law coefficient in atmospheres per mole fraction (atm/mol fraction)—enter a zero if the compound is insoluble or no Henry's Law coefficient is available

11. The LiOH removal expressed as the weight of LiOH consumed per weight of contaminant removed in lb_m LiOH/lb_m contaminant

12. The chemical group classification for the contaminant specified in appendix D of NHB 8060.1B

13. The SMAC or other threshold value expressed in milligrams per cubic meter (mg/m^3)

14. The contaminant generation rate at the inlet to device number 3 in mg/h

15. The contaminant generation rate at the inlet to device number 4 in mg/h

16. The contaminant generation rate at the inlet to device number 5 in mg/h

17. The contaminant generation rate at the inlet to device number 6 in mg/h

18. The contaminant generation rate at the inlet to device number 7 in mg/h

19. The contaminant generation rate at the inlet to device number 8 in mg/h

20. The contaminant generation rate at the inlet to device number 9 in mg/h

21. The contaminant generation rate at the inlet to device number 10 in mg/h

22. The contaminant generation rate at the inlet to device number 11 in mg/h

23. The contaminant generation rate at the inlet to device number 12 in mg/h

24. The contaminant generation rate at the inlet to device number 13 in mg/h

25. The contaminant generation rate at the inlet to device number 14 in mg/h

26. The contaminant generation rate at the inlet to device number 15 in mg/h

27. The decimal oxidation efficiency per pass for the contaminant in a high temperature catalytic oxidizer where 1.0 is fully oxidized and 0.0 is no oxidation.

Some general considerations should be noted when preparing the contaminant data input file. They are the following:

1. The molecular weights for ammonia, formaldehyde, methane, carbon monoxide, and hydrogen must be exactly 17.0, 30.03,16.04, 28.10, and 2.02 since they are used as flags in the program

2. The entire set of information, columns 1 through 27, must be input for each individual contaminant

3. Each cell in all matrices (contaminant, device, and time) must contain a value or a zero

4. The column width in all matrices (contaminant, device, and time) should be sufficient to permit at least one blank space between the column entries

5. Printing to a file should be unformatted and the range should exclude the first column (contaminant number) and any column headings

6. The file must be created in one piece without any line feeds (except at the end of a line) or carriage returns and the left margin must be set to 0 and the right margin to 240 when using Lotus 1-2-3™

7. The contaminant generation rates at the inlets of devices (columns 14 through 26) are for cases where contaminants are generated in a closed or confined space and are passed through a removal device(s) before entering the cabin (for example, a contaminant is produced in a experimental working volume and is passed through a charcoal bed before entering the cabin)

8. Some contaminant physical property data may not be available in the literature and must be estimated using correlations.

Removal Device Definition Input File Preparation

The device definition matrix, DD, contains the information which defines the removal device configuration. This information includes the type of devices, their arrangement, flow rates, and physical size or dimensions. Basic system data, such as the cabin volume, temperature, basic time increment size, convergence error specification, and the multicomponent adsorption coexistence factor, are also contained in this matrix. In addition, program data output for standard formatted data is controlled from this matrix. A sample device definition file is shown by figure 3. Data required for each of the first seven columns are the following:

1. The device number ranging from 1 through 15

2. The standard volumetric atmospheric flow through the device in cubic meters per hour (m^3/h)

Example Device Definition Data Table

USE RANGE 'LIST' DATA TABLE TO PRINT TO PRINTER
USE RANGE'DATA' TO PRINT DATA TO FILE

TCCS PROGRAM INPUT DATA
DEVICE DEFINITION TABLE

MATRIX COLUMN NO.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
DEVICE NO.	DEVICE FLOW (m3/h)	DEVICE TYPE NO.	UPSTREAM DEVICES BY NUMBER NO. 1	NO. 2	NO. 3	NOT FOR INPUT	COL 8 TO 16 USED FOR DEVICE SPECIFIC INPUTS SEE TABLE BELOW								
1	0.00	1	0	0	0	0	0	227.86	293	24	1.00E-01	1.2	0	0	0
2	0.0460	2	1	0	0	0	1	0	0	0	0	0	1	1	0
3	519.90	8	1	0	0	0	1	1.451	0	0	0	0	0	0	0
4	15.12	3	1	0	0	0	1	0.580	0.320	0	490	2	0	0	0
5	4.08	7	4	0	0	0	1	0.000	0.000	0	0	0	0	0	0
6	4.08	5	5	0	0	0	1	0.234	0.129	0	442	0	0	0	0

Example Device Definition Input File

1	0.00	1	0	0	0	0	0	227.86	293	24	1.00E-01	1.2	0	0	0
2	0.0460	2	1	0	0	0	1	0	0	0	0	0	1	1	0
3	519.90	8	1	0	0	0	1	1.451	0	0	0	0	0	0	0
4	15.12	3	1	0	0	0	1	0.580	0.320	0	490	2	0	0	0
5	4.08	7	4	0	0	0	1	0.000	0.000	0	0	0	0	0	0
6	4.08	5	5	0	0	0	1	0.234	0.129	0	442	0	0	0	0

Figure 3. Sample device definition data.

3. Device type number as defined in table 4

4. Upstream device number 1 by device number (column 1)

5. Upstream device number 2 by device number

6. Upstream device number 3 by device number

7. A zero is entered in this column for all devices since this column is used to store calculated values during the program run.

Columns 8 through 16 are specific for each device type. Data required for these columns for each device type are the following:

Table 4. Device type number and description.

Type Number	Description
1	Cabin
2	Cabin leakage
3	Axial flow charcoal bed
4	Radial flow charcoal bed
5	Lithium hydroxide bed
6	Carbon monoxide oxidizer
7	High temperature catalytic oxidizer
8	Condensing heat exchanger
9	Dummy device

Device Type Number 1: The Cabin

8. Device decimal removal efficiency equal to zero

9. Cabin atmospheric volume in cubic meters (m^3)

10. Cabin absolute temperature in kelvin (K)

11. Basic time increment in hours (h)

12. Convergence error as decimal percent (recommended values of 0.01 or 0.001)

13. Coexistence factor, approximate value of 1.20, to account for interaction or blockage of contaminants in granular activated charcoal beds

14. Cabin relative humidity (expressed as a whole number from 0 to 100 percent)

15. Not used for input therefore zero is input

16. Not used for input therefore zero is input.

Device Type Number 2: Cabin Leakage

8. Device decimal removal efficiency equal to 1.0.

Columns 9 through 16 for the leakage device are used to set standard formatted data output print switches. These columns contain either zero (0) to tell the program not to print or one (1) to tell the program to print. Print switches 1 through 5 are for diagnostic data output, and print switches 6 through 8 are for final data output. Typically, print switches 1 through 5 are set to zero during a normal simulation run.

9. Set print switch 1 to zero or one to regulate printing the contents of matrices CC and DD at the end of the precalculation setup routine, PCSET

10. Set print switch 2 to zero or one to regulate printing of the one-tenth increment convergence routine for one time increment for one contaminant (these results will be printed only if the one-tenth increment routine is used)

11. Set print switch 3 to zero or one to regulate printing of the convergence values of predicted and calculated contaminant concentration for the convergence routine CONVRG for the standard and one-twentieth time increments (useful if convergence problems occur)

12. Set print switch 4 to zero or one to regulate printing of the results for one contaminant from the main calculation routine, MCALC, after the average concentration is calculated (matrix DD and part of matrix CC for one contaminant)

13. Set print switch 5 to zero or one to regulate printing the contents of matrices DD and CC at the end of each time increment

14. Set print switch 6 to zero to print only the cabin concentration for each contaminant for each time increment or to one to print the contaminant removal rate, mass removed, and device efficiencies in addition to the cabin concentration for each time increment

15. Set print switch 7 to zero to allow form feeds between output pages or to one to suppress form feeds between output pages

16. Set print switch 8 to zero to print calculation results specified by print switch 6 at the end of the run only or to one to print calculation results at the end of each time increment.

Device Type Number 3: Axial Flow Charcoal Bed

8. Maximum device decimal removal efficiency equal to 1.0

9. Charcoal bed length in meters (m)

10. Charcoal bed diameter in meters (m)

11. Not used for input and set to 0

12. Charcoal bulk density in kilograms per cubic meter (kg/m^3)

13. Charcoal bed treatment type (1 for chromate treated charcoal for formaldehyde removal, 2 for phosphoric acid treated charcoal for ammonia removal, or 0 for untreated charcoal)

14. Time of first regeneration in hours (h)

15. Time interval between each regeneration in hours (h)

16. Regeneration duration in hours (h).

Device Type Number 4: Radial Flow Charcoal Bed

8. Maximum device decimal removal efficiency equal to 1.0

9. Radial flow bed length in meters (m)

10. Radial flow bed outside diameter in meters (m)

11. Radial flow bed inside diameter in meters (m)

12. Charcoal bulk density in kilograms per cubic meter (kg/m^3)

13. Charcoal bed treatment type (1 for chromate treated charcoal for formaldehyde removal, 2 for phosphoric acid treated charcoal for ammonia removal, or 0 for untreated charcoal)

14. Time of first regeneration in hours (h)

15. Time interval between each regeneration in hours (h)

16. Regeneration duration in hours (h).

Device Type Number 5: LiOH Bed

8. Maximum device decimal removal efficiency equal to 1.0

9. LiOH bed length in meters (m)

10. LiOH bed diameter in meters (m)

11. Not used for input and set to 0

12. LiOH bulk density in kilograms per cubic meter (kg/m^3)

13. Time of first changeout in hours (h)

14. Time between changeouts in hours (h)

15. Not used for input and set to 0

16. Not used for input and set to 0.

Device Type Number 6: Ambient Temperature CO Oxidizer

8. Maximum device decimal removal efficiency equal to 1.0

9. Oxidizer bed length in meters (m)

10. Oxidizer bed diameter in meters (m)

11. Not used for input and set to 0

12. Not used for input and set to 0

13. Not used for input and set to 0

14. Not used for input and set to 0

15. Not used for input and set to 0

16. Not used for input and set to 0.

Device Type Number 7: High Temperature Catalytic Oxidizer

8. Maximum device decimal removal efficiency equal to 1.0

9. Not used for input and set to 0

10. Not used for input and set to 0

11. Not used for input and set to 0

12. Not used for input and set to 0

13. Not used for input and set to 0

14. Not used for input and set to 0

15. Not used for input and set to 0

16. Not used for input and set to 0.

Device Type Number 8: Condensing Heat Exchanger

8. Maximum device decimal removal efficiency equal to 1.0

9. Condensate flow rate in kilograms per hour (kg/h)

10. Not used for input and set to 0

11. Not used for input and set to 0

12. Not used for input and set to 0

13. Not used for input and set to 0

14. Not used for input and set to 0

15. Not used for input and set to 0

16. Not used for input and set to 0.

Device Type Number 9: The Dummy Device

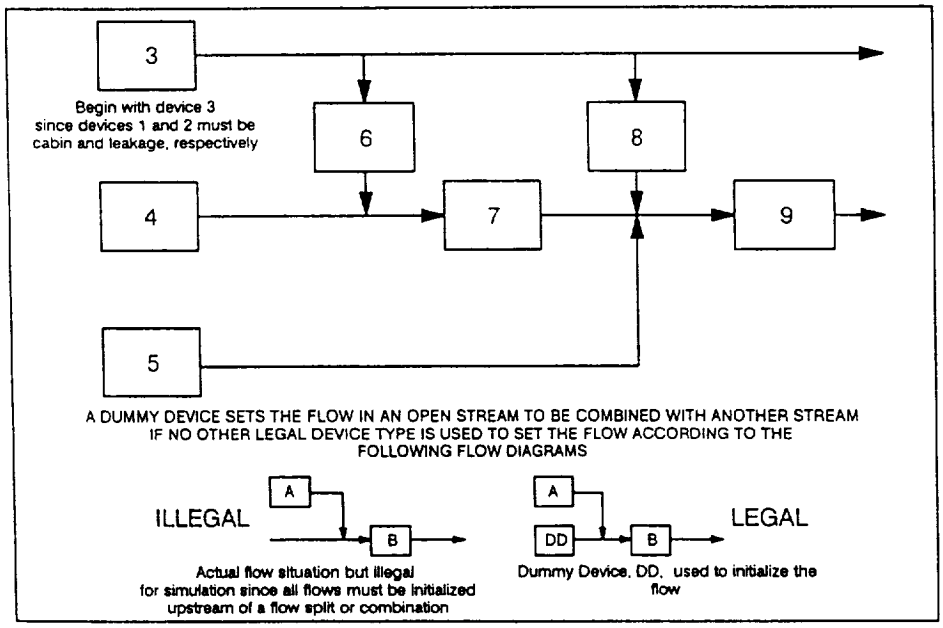
The dummy device serves to set the flow rate through a line when combining or splitting flows between upstream and downstream devices. Legal and illegal dummy device use is illustrated at the bottom of figure 4. When combining or splitting streams, dummy devices are required to set the upstream flow rates being combined or split.

8. Maximum device decimal removal efficiency equal to 0

9. Not used for input and set to 0

10. Not used for input and set to 0

11. Not used for input and set to 0



NOTE: NUMBERS INDICATE THE DEVICE NUMBER, NOT THE DEVICE TYPE AND BEGIN WITH 3 SINCE CABIN AND LEAKAGE ARE DEVICE NUMBERS 1 AND 2 FOR ANY SIMULATION.

Figure 4. Sample device configurations and dummy device use.

12. Not used for input and set to 0

13. Not used for input and set to 0

14. Not used for input and set to 0

15. Not used for input and set to 0

16. Not used for input and set to 0.

Removal Device Arrangement Rules

Some simple rules apply to arranging removal devices in the removal device definition file. These rules are the following:

1. The first device must always be the cabin device type 1

2. The second device must always be the leakage device type 2

3. Device numbers 3 through 15 may be any legal device type

4. Devices must be numbered so that calculations for upstream devices occur before calculations for downstream devices since calculations are sequential by the device number specified in column 1

5. Inlet flow rates must be specified for each device to allow proper inlet concentration calculation for split flows

6. If the cabin is upstream of any device, column 4 should indicate this by entering a 1.

Figure 4 shows a sample device configuration along with some legal and illegal device configurations.

Removal Device Regeneration

Regeneration of the axial and radial flow charcoal beds and the LiOH bed are accomplished by entering the appropriate regeneration information into matrix DD. Columns 14, 15, and 16 are used for regenerating the axial and radial charcoal beds and should contain the first time in hours from the beginning of the run that regeneration occurs (note that the run begins at zero hours and the run time increments itself according to the basic time increment), the time in hours between each regeneration, and the time required to regenerate the bed in hours. Columns 13 and 14 are used for LiOH bed regeneration and should contain the first changeout time in hours and the time between each change out in hours, respectively. No regeneration duration is required for the LiOH bed. It is important that the time between each regeneration or changeout and the regeneration time must be equal to or an even multiple of the basic time increment for the calculation. If they are not, the program will truncate them. Rules to be followed when simulating a regenerable bed are the following:

1. The initial regeneration time, changeout or regeneration interval, and time to regenerate must be multiples of the basic time increment specified in the device definition matrix row 1 column 11.

2. If the values are not even multiples of the time increment, they will be truncated to the next smallest multiple which could be zero.

3. If the regeneration duration desired is less than one time increment, the input flow rate can be modified manually in the program input according to the following:

$$Q_{mod} = Q_{actual} \times \{ 1 - (\tau_{reg\ duration} / \tau_{reg\ interval}) \} . \quad (1)$$

The modified flow rate should be input in the device definition matrix column 2 for that device. the regeneration duration should then be set to zero. If the flow rate is changed during the simulation, it may be necessary to add a dummy device in parallel with the regenerating device so that the original flow rate may be supplied to any possible downstream devices.

4. For no regeneration, set the regeneration interval equal to zero.

Time-Dependent Data Input File Preparation

During a simulation run, it is possible to change the generation rate of any contaminant both in the cabin or for any device which is operating. Device flow rates and other device information such as the cabin volume, the cabin temperature, and basic time increment may also be changed. Time-dependent changes are accomplished by using the time-dependent data matrix, TT. This matrix contains seven columns for each row. Each line in matrix TT does not allow simultaneous contaminant generation rate and device definition data changes. For example, the flow rate and contamination generation rate cannot be changed using a single line. Each change must have its own unique change line. However, two simultaneous device definition changes may be made for a single removal device using one time change file line. Table 5 shows the heading for the time-dependent data table and six common cases for time-dependent data changes. An example time-dependent data file is shown by the seven columns under the data heading of table 6. The time-dependent data file read by the program is created by selecting only the time change numbers when writing the data to the file. The heading should not be included in the data file. If it is, the program will write an error message to the screen telling the user that the data file cannot be read. Each time-dependent file may contain up to 750 lines of changes. Rules for using this data file are the following:

General Time-Dependent Change Rule

1. Column 1 contains the change time in hours for all changes. Any update can occur only at the beginning of a time increment. If a change time is not an exact multiple of the basic time increment, the time will be truncated to the next lowest multiple of the increment.

Changing Contaminant Generation Rates

1. Column 1 contains the change time in hours (h).

2. Column 2 contains the contaminant sequential number to be changed. The contaminant number must be greater than or equal to one, and less than or equal to the maximum number of contaminants in the contaminant input file.

3. Column 3 contains the new or changed generation rate.

Table 5. Several common time-dependent changes.

Type of Change	Change Items						
Time-Dependent Data Table Sample Heading	FILE:TCTT02 28-May 1992 TIME DEPENDENT CONTAMINANT INPUT DATA FILE (MAT TT) MAKE SURE ALL CELLS HAVE VALUE OR 0 IN CELL USE RANGE 'LIST' TO PRINT TO PRINTER USE RANGE 'DATA' TO PRINT TO FILE ========== CHANGE CONT GEN IN MAT CDI <----------> CHANGE DEVICE FLOW RATE IN MAT DD <----------> CHANGE OTHER MAT DD INFO <----------> CHANGE TIME (h) / CONT NO. / CONT GEN RT (mg/h) / DEVICE NO. / NEW Q DEVICE (m^3/h) / MAT DD COLUMN NO. / NEW VALUE						
1. No changes	0	0	0	0	0	0	0
2. Change contaminant generation rate	24	1	800	1	-1	-1	-1
3. Change device flow rate	24	-1	-1	3	15	-1	-1
4. Change cabin volume	24	-1	-1	1	-1	9	150
5. Change device flow rate and bed length	24	-1	-1	3	15	9	1.5
6. Change time increment	24	-1	-1	1	-1	11	1

Table 6. A sample time-dependent data input file.

Change Type	Data to be Read by the Computer Program						
Change increment	720	-1	-1	1	-1	11	1
Change flow	720	-1	-1	3	4.8	-1	-1
Change flow	720	-1	-1	4	4.8	-1	-1
Change flow	720	-1	-1	5	4.8	-1	-1
Change increment	732	-1	-1	1	-1	11	6
Change increment	768	-1	-1	1	-1	11	5
Change increment	773	-1	-1	1	-1	11	23
Change flow	773	-1	-1	3	0	-1	-1
Change flow	773	-1	-1	4	0	-1	-1
Change flow	773	-1	-1	5	0	-1	-1
Change increment	796	-1	-1	1	-1	11	24
Change increment	844	-1	-1	1	-1	11	2
Change flow	846	-1	-1	3	4.8	-1	-1
Change flow	846	-1	-1	4	4.8	-1	-1
Change flow	846	-1	-1	5	4.8	-1	-1
Change flow	846	-1	-1	6	281	-1	-1
Change generation	846	5	0.1274	1	-1	-1	-1
Change generation	846	8	3.4825	1	-1	-1	-1
Change generation	846	13	3.5398	1	-1	-1	-1
Change generation	846	14	2.8109	1	-1	-1	-1
Change generation	846	22	0.3228	1	-1	-1	-1
Change generation	846	27	0.6651	1	-1	-1	-1
Change generation	846	121	14.9589	1	-1	-1	-1
Change generation	846	137	4.2861	1	-1	-1	-1
Change generation	846	149	0.0075	1	-1	-1	-1
Change generation	846	153	39.6206	1	-1	-1	-1
Change generation	846	154	6.5515	1	-1	-1	-1
Change generation	846	155	2.1837	1	-1	-1	-1
Change increment	892	-1	-1	1	-1	11	24

4. Column 4 contains the removal device number whose contaminant generation rate is to be changed. The device number must be greater than or equal to 1 and less than or equal to the maximum number of devices in the simulation. (Device 2 may be used, but it does not effect the calculation since any change would be canceled out by the 100-percent removal efficiency provided by cabin leakage.)

5. Column 5 is ignored and is set equal to -1.

6. Column 6 is ignored and is set equal to -1 Column 7 is ignored and is set equal to -1.

Changing Device Definition Matrix Information

1. Column 1 contains the change time in hours (h).

2. Column 2 is ignored and is set equal to -1.

3. Column 3 is ignored and is set equal to -1.

4. Column 4 contains the device number and must be greater than or equal to 1 and less than or equal to the maximum number of removal devices.

5. Column 5 contains the new device definition matrix information. This information must be greater than zero if a change is desired. If no input is desired, use -1 since this will prevent the program from reading the new information in column 7.

6. Column 6 contains the device definition matrix column number that the change is to occur and must be greater than or equal to zero and less than or equal to 16. Any other value in this column causes the program to ignore the value in column 7.

7. Column 7 contains the new device definition matrix value. Both the flow rate and any other device change can be made simultaneously for any device.

A time-dependent data file is necessary for program execution even when no time-dependent changes will be made. In this case, a single row with all the columns set equal to zero is required for the time-dependent data file.

IBM and Compatible Program Version Execution

Once the three input files have been prepared, the TCCS computer program is ready to be executed. Execution is initiated by typing TCCS at the DOS prompt. If a very large contaminant data file will be used for the simulation and contaminant plot data that will be obtained during the run, the program should be executed by typing TCCS /R 10000 to allow for larger output records during the run. The number used with the "R" option can range between 512 and 65,527 and corresponds to record lengths of 512 b to 65,527 b. Normal execution without the "/R" option results in the default record length of 1,024 b.

It is important that the terminal keyboard is in the CAPS LOCK mode since the program only reads capitalized alphanumerics during interactive input. A carriage return is entered from the keyboard after responding to each prompt. If inappropriate information is entered, or a file with the incorrect format is specified, the program will indicate that an error reading the file has occurred and will prompt the user for the desired information again.

Reading Input Data

The program begins by prompting the user for the names of the input files to be used for the simulation. A prompt is written to the screen asking for each file name beginning with the contaminant data input file. The file name is entered by typing the file path, the filename, and its extension. This allows the program to read the files if they are stored on the computer disk in a separate directory or allows the program to access the files from a floppy diskette. If the files are in the same directory as the program executable file, then no path designation is necessary. The removal device definition file is read next followed by the time-dependent data file.

After each file has been read successfully, the program writes a message to the screen indicating that the data file has been read. Also, after each file has been read, the program prompts the user for a decision concerning input file data output by writing a prompt to the screen requesting whether the data

file that has just been read should be printed. The user should respond to this prompt with a "Y" or an "N." The "Y" response results in a second prompt for the user to designate how the data file should be printed. The choices are the printer (LPT1), the computer screen (CON), or neither (END). This option is available for the user to view the contents of each data file to make sure the data is correct before the program calculation routine begins. Usually, this option is not necessary if the input files have been created carefully. The "N" response causes the program to move to the next input data prompt.

Once data file input is completed, the program prompts the user for the mission duration in hours. This is the length of time that the particular mission being simulated will last. For example, a 7-d Spacelab mission duration is 168 h and the number 168.0 should be entered at this prompt.

Data Output Decisions

After the data files and mission duration have been read by the program, the user is prompted for a decision on calculation data output. The TCCS computer program is capable of producing output data in several formats and writing these data to multiple output devices. The principal output data consist of standard formatted output data controlled by the print switches defined in the device definition data file and plot data output which is specified interactively by the user for each program execution. The program prompts the user for decisions concerning plot data output and output devices in the following order.

Concentration and Device Efficiency Plot Data Output. Concentration data and removal device efficiency data for each basic time increment can be output to two separate data files. The user is prompted by the program for a decision to output only concentration data, only efficiency data, both concentration and efficiency data, or neither. The user selects this options by entering "C," "E," "B," or "N," respectively, at the prompt. Examples of the data output for both concentration and efficiency plot data are shown by tables 7 and 8.

Table 7. Example concentration plot data output.

Initial Time (h)	Final Time (h)	Concentration (mg/m^3)				
		Cont. 1	Cont. 2	Cont. 3	Cont. 4	Cont. n
0.000	1.000	1.189	0.2432E–03	0.1339	0.1899....	0.2022E–1
1.000	12.000	10.16	0.2077E–02	1.464	1.308	0.2201
12.000	24.000	14.72	0.3012E–02	2.655	1.637	0.3972

Toxic Hazard Index Output. The toxic hazard index is a technique used by toxicologists to determine the toxicological acceptability for a mixture of chemical compounds in the atmosphere. It is analogous to a SMAC in some respects. The overall toxic hazard index is the summation of the ratios of each contaminant's atmospheric concentration to its SMAC. Ideally, this summation should be less than one. A more detailed definition of the toxic hazard index is found in the appendix and reference 12.

The user is prompted by the program for a decision to write the toxic hazard index to the standard formatted output device, to the standard output device and a plot data file, or neither. Each option is selected by entering "Y," "P," or "N" at this prompt.

Table 8. Example removal device efficiency plot data output.

Initial Time	Final Time	Device	Efficiency for Each Contaminant								
			1	2	3	4	5	6	7	8	n
0.00	1.00	2	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.00	1.00	3	0.000	0.000	0.000	0.021	0.125	0.116	1.000	0.000	0.000
0.00	1.00	4	1.000	1.000	0.056	1.000	1.000	1.000	1.000	0.000	0.000
0.00	1.00	5	0.330	1.000	0.950	1.000	1.000	1.000	1.000	1.000	1.000
0.00	1.00	6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	7	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	14	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.00	1.00	15	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	2	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
1.00	12.00	3	0.000	0.000	0.000	0.021	0.125	0.116	1.000	0.000	0.000
1.00	12.00	4	1.000	1.000	0.003	1.000	1.000	1.000	1.000	0.000	0.000
1.00	12.00	5	0.330	1.000	0.950	1.000	1.000	1.000	1.000	1.000	1.000
1.00	12.00	6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	7	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	14	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.00	12.00	15	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	2	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
12.00	24.00	3	0.000	0.000	0.000	0.021	0.125	0.116	1.000	0.000	0.000
12.00	24.00	4	1.000	1.000	0.002	1.000	1.000	1.000	1.000	0.000	0.000
12.00	24.00	5	0.330	1.000	0.950	1.000	1.000	1.000	1.000	1.000	1.000
12.00	24.00	6	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	7	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	8	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	9	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	10	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	11	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	12	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	13	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	14	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
12.00	24.00	15	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Standard Formatted Output. Standard formatted calculation data produced by the program can be output to a data file, the printer, the screen, or none of these options. The data file option requires the user to input the path, file name, and extension of a file that the program will open and write calculation data to during the execution. Again, the path is necessary only if the data file is not in the same directory as the program executable file. The program checks the file name to determine whether the file already exists. If the file exists, the program indicates this on the screen and asks the user whether it should be overwritten. The user responds to this prompt by entering "Y" or "N." The "Y" response allows overwriting the present contents of the file and the "N" response causes the program to prompt the user for another file name. The printer selection is made by entering LPT1 at this prompt and results in formatted calculation data output to the print device for the computer. This option is recommended only if output is desired at the end of the program execution since large quantities of paper are produced. The screen option is selected by entering CON and results in the formatted data to be written to the screen. The data scrolls by rapidly when the CON option is selected, and scrolling may be stopped by holding down the control key and pressing the S key (CTRL S). Scrolling is restarted by typing CTRL S again. The END option terminates program execution. The program is designed to ask the user if any other cases will be run before terminating execution. The END option causes this prompt to be written to the screen and the user responds by entering "Y" or "N." The "Y" response reinitializes the program and the user is prompted for new input data. The "N" response terminates execution completely.

WARNING: Be careful to specify LPT1, CON, or END when making data output decisions to send data to the printer, the screen, or to reset the program. Any other response will cause the data to be written to a file.

Plot Data File Designation

After the output selections have been made, the program prompts the user for file names for each of the plot data files. A separate file is created for concentration plot data, device removal efficiency plot data, and toxic hazard index plot data. Prompts for each file name are written to the screen only if the user has chosen the options specifying these data for the particular program execution run. As with the standard output device, the user responds to this prompt by entering the path, filename, and extension. The path is not necessary if the file is in the same directory as the program executable file. The program checks to see if the file already exists. If this file exists, the program writes a prompt to the screen asking the user if the file should be overwritten. The user must respond to this prompt by entering a "Y" or "N." The "Y" response opens the file and permits overwriting, while the "N" response causes the program to prompt the user for a new file name.

Calculation Routine Execution

After completing the input and output designations, the program begins the calculation routine. During this routine, information will be written to the computer screen depending on the output selections made. Standard formatted output for each time increment will be written to the screen if print switch 8 in the device definition data file is set to 1 and the CON option for output has been selected. However, if print switch 8 is set to 1 and the LPT1 or file option has been selected, only the increment number and the increment starting and ending times will be written to the screen. Similarly, if print switch 8 is set to 0 and any standard output device selection has been made, the program will write only the increment number and the increment starting and ending times to the screen during the calculation routine. At the end of the calculation routine, the CON output option instructs the program to write the final standard formatted output data to the screen, the LPT1 option sends these data to the printer, and the file option sends the data to the designated file.

During execution, the program may also write error messages to the screen. Most error messages relate to output devices and cause the data to not be written to the specified data file. The program indicates the location of the error in the execution and will continue to execute unless the disk capacity has been exceeded. In this case, the execution terminates.

A second type of warning is written to the screen when the calculation for a contaminant does not converge. This warning indicates a serious problem where the concentration and efficiency calculations for a contaminant did not converge to within the specified convergence error within 20 iterations using the basic time increment and 20 iterations using one-twentieth the basic time increment. The program will continue to execute; however, the results for that contaminant will be incorrect. This problem is corrected by either using a smaller basic time increment or increasing the convergence error specified in the device definition data file.

After the calculation routine is complete, the program writes a prompt to the screen asking the user if more cases will be run. The user responds to this prompt by entering "Y" or "N." The "Y" response causes the program to loop to the data entry routine to allow the user to specify input files for the next case. The "N" response terminates the program execution and the DOS prompt will appear on the screen.

Output Data File Manipulation

The program is capable of producing up to four output data files during a single execution. These files contain the standard formatted output, concentration plot data, device removal efficiency plot data, and toxic hazard index plot data. All of these files are in ASCII format and can be loaded into commercially available word processing and spreadsheet programs for editing and analysis. Specific guidelines for manipulating these files are described.

Standard Formatted Output

The data file containing the standard formatted output may be loaded into a word processing program to be included in a report or memorandum. The format may be edited in the program to suit the user's needs. The font size may have to be reduced to fit on 8.5 by 11 inch paper in the portrait orientation. The landscape orientation is recommended. An example of the standard formatted output is shown by figure 5.

Concentration Plot Data

Concentration plot data consists of the beginning and ending time for each time increment and the concentration for each contaminant in the simulation at the end of the time increment. An example of concentration plot data output is shown by table 7. The data are arranged in columns according to the following:

1. The first column contains the increment beginning time in hours (h)

2. The second column contains the increment ending time in hours (h)

3. All columns beyond the first two contain the sequential (contaminant 1 through n) contaminant concentration for each contaminant in milligrams per cubic meter (mg/m^3).

1

PROGRAM VERSION 8.0 Alpha 04-10-92

5/27/1992 14:51 SAMPLE.DAT PAGE 1
TIME INCR 1 INITIAL TIME (HRS)= 0.00 FINAL TIME (HRS)= 1.00

CONT NO.	NAME	FINAL CABIN CONC (MG/M3)	MAC	EXCEEDS MAC
1	1,1,2-triCl-1,2,2-triFlethane	1.189	383.0	N
2	1,3-Butadiene	0.2432E-03	221.2	N
3	Methane	0.1339	1771.	N
4	2-butanone	0.1899	59.00	N
5	1-benzo[b]pyrrole	0.3853E-02	0.4800	N
6	methyl hydrazine	0.1093E-03	0.8000E-01	N
7	Ammonia	0.9042E-01	17.40	N
8	Carbon monoxide	0.1046	28.60	N
9	Hydrogen	0.2022E-01	247.3	N

GROUP T-VALUES AS SPECIFIED IN NHB 8060.1B APPENDIX D

-01-	-02-	-03-	-04-	-05-	-06-	-07-	-08-	-09-	-10-	-11-	-12-	-13-	-14-	-15-	-16-
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01

OVERALL T-VALUE
0.01

1

5/27/1992 14:51 SAMPLE.DAT PAGE 2
TIME INCR 1 INITIAL TIME (HRS)= 0.00 FINAL TIME (HRS)= 1.00

RATE OF CONTAMINANT REMOVAL-EACH DEVICE (MG/HR) SHEET 1

NO.	NAME	CABIN	LEAK	DEV3	DEV4	DEV5	DEV6	DEV7	DEV8
1	1,1,2-triCl-1,2,2-triFlethane	270.9	0.2765E-01	0.4108E-04	9.087	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	1,3-Butadiene	0.5541E-01	0.5655E-05	0.9341E-07	0.1859E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	Methane	30.50	0.3089E-02	0.3489E-05	0.5648E-01	0.2458	0.0000E+00	0.0000E+00	0.0000E+00
4	2-butanone	43.27	0.4452E-02	1.069	1.463	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5	1-benzo[b]pyrrole	0.8779	0.9381E-04	0.1328	0.3084E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6	methyl hydrazine	0.2490E-01	0.2652E-05	0.3483E-02	0.8718E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7	Ammonia	20.60	0.2827E-02	31.96	0.9293	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8	Carbon monoxide	23.83	0.2413E-02	0.1521E-05	0.7547E-08	0.2140	0.0000E+00	0.0000E+00	0.0000E+00
9	Hydrogen	4.608	0.4666E-03	0.2861E-06	0.1359E-13	0.4138E-01	0.0000E+00	0.0000E+00	0.0000E+00

Figure 5. Example standard formatted data output.

1

5/27/1992 14:51 SAMPLE.DAT PAGE 3

TIME INCR 1 INITIAL TIME (HRS)= 0.00 FINAL TIME (HRS)= 1.00

TOTAL CONTAMINANT MASS REMOVED BY EACH DEVICE (MG) SHEET 1

NO.	NAME	CABIN	LEAK	DEV3	DEV4	DEV5	DEV6	DEV7	DEV8
1	1,1,2-triCl-1,2,2-triFlethane	270.9	0.2765E-01	0.4108E-04	9.087	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	1,3-Butadiene	0.5541E-01	0.5655E-05	0.9341E-07	0.1859E-02	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	Methane	30.50	0.3089E-02	0.3489E-05	0.5648E-01	0.2458	0.0000E+00	0.0000E+00	0.0000E+00
4	2-butanone	43.27	0.4452E-02	1.069	1.463	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5	1-benzo[b]pyrrole	0.8779	0.9381E-04	0.1328	0.3084E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
6	methyl hydrazine	0.2490E-01	0.2652E-05	0.3483E-02	0.8718E-03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
7	Ammonia	20.60	0.2827E-02	31.96	0.9293	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
8	Carbon monoxide	23.83	0.2413E-02	0.1521E-05	0.7547E-08	0.2140	0.0000E+00	0.0000E+00	0.0000E+00
9	Hydrogen	4.608	0.4666E-03	0.2861E-06	0.1359E-13	0.4138E-01	0.0000E+00	0.0000E+00	0.0000E+00

1

5/27/1992 14:51 SAMPLE.DAT PAGE 4

TIME INCR 1 INITIAL TIME (HRS)= 0.00 FINAL TIME (HRS)= 1.00

DEVICE REMOVAL EFFICIENCY AT END OF TIME INCREMENT (DEC)

NO.	NAME	#2	#3	#4	#5	#6	#7	#8	#9	#10	#11	#12	#13	#14	#15
1	1,1,2-triCl-1,2,2-triFlethane	1.000	0.000	1.000	0.330	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	1,3-Butadiene	1.000	0.000	1.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3	Methane	1.000	0.000	0.056	0.950	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
4	2-butanone	1.000	0.021	1.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5	1-benzo[b]pyrrole	1.000	0.125	1.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
6	methyl hydrazine	1.000	0.116	1.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7	Ammonia	1.000	1.000	1.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8	Carbon monoxide	1.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
9	Hydrogen	1.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Figure 5. Example standard formatted data output (continued).

These data can be loaded into a spreadsheet program (Lotus 1-2-3™ is recommended) and the appropriate ranges selected for preparing plots of concentration as a function of time.

Efficiency Plot Data

Removal device efficiency data consist of the beginning and ending time for each increment, the removal device number (2 through 15), and the decimal of each device for each contaminant for that time increment. This data file is arranged as a square matrix in which each time increment has 14 rows as shown by table 8. Each row corresponds to a removal device and contains columns which include the following:

1. The first column contains the increment beginning time in hours (h)
2. The second column contains the increment ending time in hours (h)
3. The third column contains the removal device number (dimensionless)
4. All columns beyond the first three contain the sequential contaminant removal efficiency for that device for each individual contaminant (contaminant 1 through n).

It must be noted that the cabin, designated as device number 1, is not included since cabin removal efficiency is not relevant. These data can be loaded into a spreadsheet program and then sorted by the removal device number column and the time increment ending time column to obtain a time-dependent removal device efficiency profile for each removal device. The appropriate data ranges may then be selected for producing data plots.

Toxic Hazard Index Data

Toxic hazard index data consist of the beginning time, ending time, and overall toxic hazard index calculation for each time increment. These data, as shown by table 9, are arranged in three columns which include the following:

1. The first column contains the increment beginning time in hours (h)
2. The second column contains the increment ending time in hours (h)
3. The third column contains the overall toxic hazard index (dimensionless).

These data can be loaded into a spreadsheet program and the second and third columns selected as the plot data ranges.

Table 9. Example toxic hazard index plot data output.

Initial Time	Final Time	Hazard Index
0.00	1.00	0.01
1.00	12.00	0.07
12.00	24.00	0.11

Macintosh™ Program Version Execution

The Macintosh™ program version execution is much more simple than the IBM and compatible program version. Execution is started by positioning the cursor over the TCCS computer program application icon, shown in figure 6, and double clicking with the mouse. The program displays the program banner which contains the program name, version number, and version date and then prompts for the input data. At this prompt, a standard Macintosh™ file location window is displayed, as shown in figure 7, and the appropriate file is selected by highlighting the file name with the cursor and double clicking with the mouse on the open bar to the right. Similar windows appear for selecting the device definition and time-dependent data files.

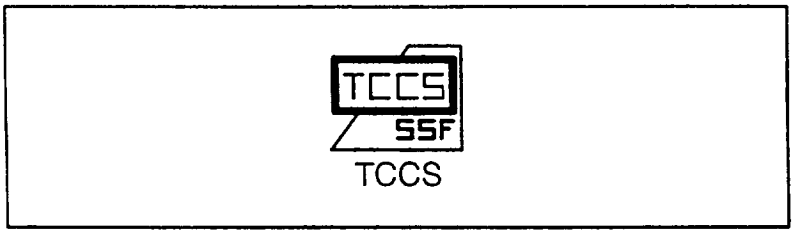


Figure 6. Macintosh™ program version application icon.

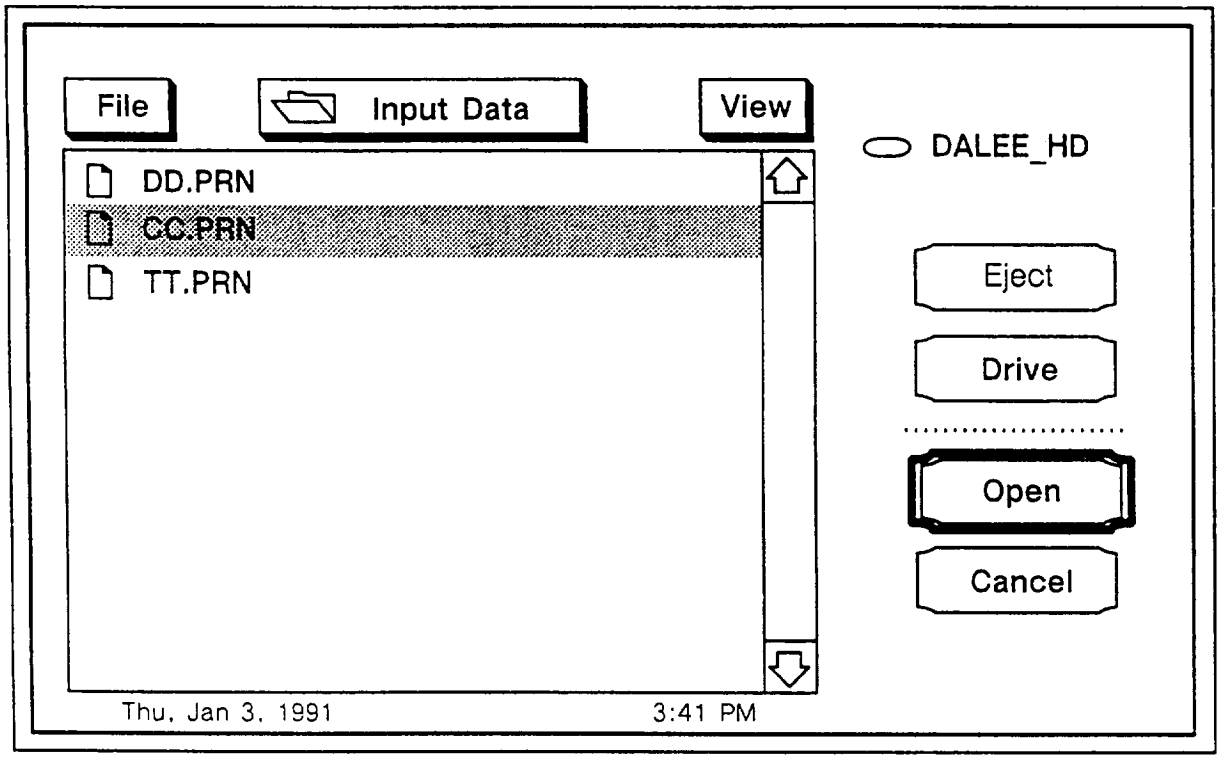


Figure 7. Example Macintosh™ file selection window.

After the three input files have been located, the main user input screen appears as shown in figure 8. The user enters the mission duration time and selects options to write the run time data to the screen, files, or both by positioning the cursor in the appropriate box and clicking with the mouse. When the user is finished with this screen, the cursor is positioned over the "OK" box and clicked with the mouse. If any of the data are to be sent to a file, the program prompts for the file name with a standard Macintosh™ pop-up window similar to the illustration in figure 9.

The final step before the program begins the main calculation routine is to name the plot data output files for concentration and device removal efficiency data. This is accomplished with the standard Macintosh™ pop-up window shown in figure 9.

Program solution is initiated after designating the plot files, and upon completion, the user is asked by the program if another run is desired. The user responds to this prompt by typing "yes" or "no." A "yes" response reinitializes the program and prompts the user for new input and output files. A "no" response terminates the program execution, and the user may then quit the application or return to the Macintosh™ Finder. From the Finder, data plotting applications may be selected to analyze the program's concentration and device efficiency data.

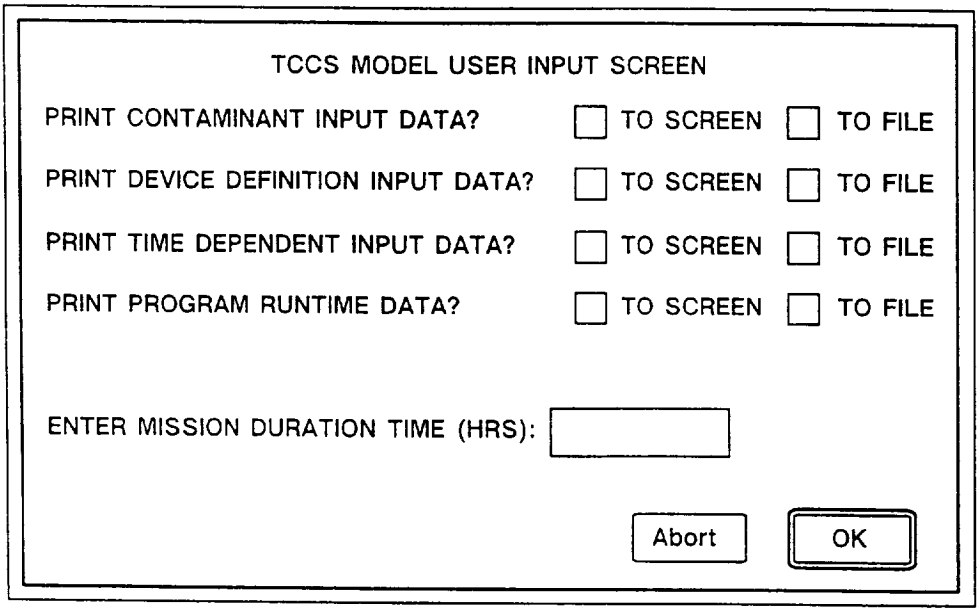


Figure 8. TCCS computer program user input screen.

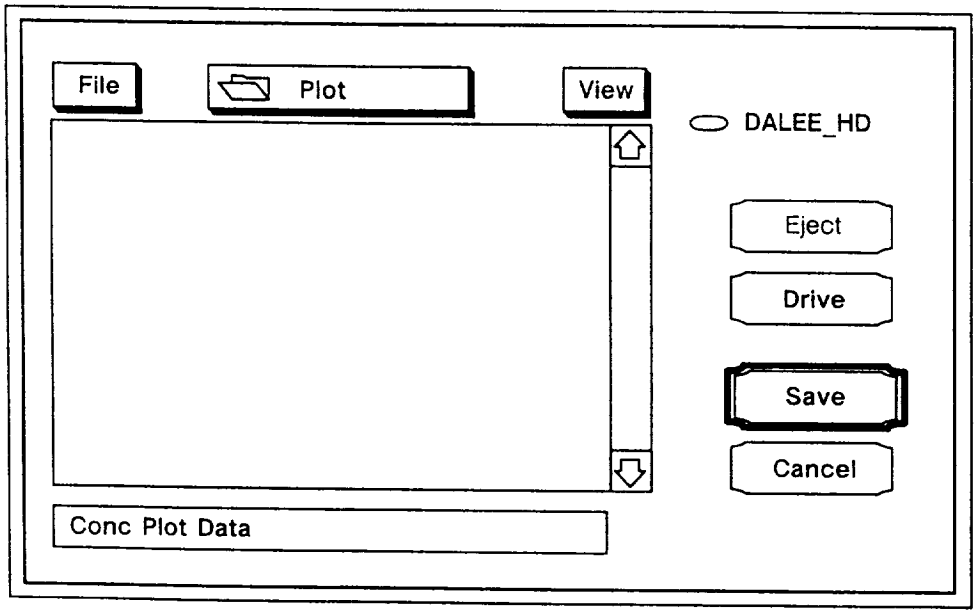


Figure 9. Window for naming plot data output files.

APPENDIX

TOXIC HAZARD INDEX DESCRIPTION

The toxic hazard index, or T-value, is the method used by toxicologists to assess the acceptability of an atmosphere containing a mixture of contaminants. This approach is derived from the American Conference of Governmental Industrial Hygienists guidelines for setting threshold limit values for contaminant mixtures. Since the effects on humans of many atmospheric contaminants are considered to be additive, this mixture approach is applied to 16 contaminant groups. The groups considered in the T-value calculation used in the TCCS computer program are the following:

1. Alcohols
2. Aldehydes
3. Aromatic hydrocarbons
4. Esters
5. Ethers
6. Chlorocarbons
7. Chlorofluorocarbons
8. Fluorocarbons
9. Hydrocarbons
10. Inorganic acids
11. Ketones
12. Mercaptans and sulfides
13. Nitrogen oxides
14. Organic acids
15. Organic nitrogens
16. Miscellaneous.

The group numbers used in the computer program output correspond to the above group listing.

The T-value is calculated for each group by calculating the sum of the ratios of the contaminants' concentrations to their maximum allowable concentration, while the overall T-value is the sum of the group T-values for the alcohols, aldehydes, aromatic hydrocarbons, esters, ethers, hydrocarbons,

inorganic acids, ketones, nitrogen oxides, organic acids, and miscellaneous groups. These calculations are conducted according to the following equations:

$$T_{group} = \Sigma\, C_c/C_m\,, \tag{A1}$$

$$T_{overall} = \Sigma\, T_{group}\,, \tag{A2}$$

where C_c is the contaminant concentration in the atmosphere in mg/m^3 and C_m is the maximum allowable concentration in the atmosphere in mg/m^3.

The criteria for acceptability are the following:

1. The T-value for each group must be less than one

2. The overall T-value must be less than one.

If either of these criteria are exceeded, the atmosphere is considered unacceptable.

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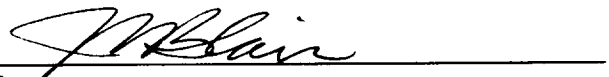
APPROVAL

A USERS' GUIDE TO THE TRACE CONTAMINANT CONTROL SIMULATION COMPUTER PROGRAM

By J.L. Perry

The information in this report has been reviewed for technical content. Review of any information concerning Department of Defense or nuclear energy activities or programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.



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